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Microscopic Approaches to Nuclear Structure: Configuration Interaction

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Abstract. The configuration interaction (CI) approach to solving the nuclear many-body problem, also known as the interacting shell model, has proven to be powerful tool in understanding the structure of nuclei. The principal criticism of past applications of the shell model is the reliance on empirical tuning to interaction matrix elements. If an accurate description of nuclei far from the valley of stability, where little or no data is available, a more fundamental approach is needed. This starts with recent ab initio approaches with effective interactions in the no-core shell model (NCSM). Using effective-field theory for guidance, fully ab initio descriptions of nuclei up to ^{16}O with QCD based NN, NNN, and NNNN interactions will be possible within the next five years. An important task is then to determine how to use these NCSM results to develop effective interactions to describe heavier nuclei without the need to resort to an empirical retuning with every model space. Thus, it is likely that more traditional CI applications utilizing direct diagonalization and more fundamental interactions will be applicable to nuclei with perhaps up to one hundred constituents. But, these direct diagonalization CI applications will always be computationally limited due to the rapid increase in the number of configurations with particle number. Very recently, the shifted-contour method has been applied to the Auxiliary-field Monte Carlo approach to the Shell Model (AFMCSM), and preliminary applications exhibit a remarkable taming of the notorious sign problem. If the mitigation of the sign problem holds true, the AFMCSM will offer a method to compute quantum correlations to mean-field applications for just about all nuclei; giving exact results for CI model spaces that can approach 10^{20-25}. In these lectures, I will discuss modern applications of CI to the nuclear many-body problem that have the potential to guide nuclear structure theory into the next decade.

1 Introduction

A fully microscopic description of the properties of atomic nuclei, especially from first principles, has been a long-standing goal in nuclear structure theory. Primarily because of the nature of the interaction between the constituent nucleons, this is an extraordinarily difficult problem that is only now beginning to be realized. This realization is coming about because of two reasons. The first is the advent of new theoretical methods such as Green's Function Monte Carlo (GFMC) [1] and effective interaction theory utilized in the No-core shell model (NCSM) [2, **?**], which allow a more complete treatment of the fundamental inter-nucleon interactions in a many-body system. The second, and perhaps more important reason, is the enabling capability provided by modern super computers. Indeed, I believe we now are poised at the cusp of a revolution in the treatment of the quantum many-body problem. The deployment of modern supercomputers will likely permit exact first-principles solutions for all nuclei up to Oxygen, and selected nuclei near

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closed shells (with coupled-cluster methods [4]), within the next decade. More important in the broader context is that these studies will lead to an improved understanding of the effective interaction required in many-body systems so that similar fundamental studies can be performed on heavier nuclei across the chart of the nuclides.

The fundamental importance of atomic nuclei is manifested in their ubiquitous presence in the universe and their special representation of the quantum many-body problem. Nuclei make up most of the visible matter in the universe, and reactions between them are the dynamos that power the stars. In addition, one of the top questions in science today is how the elements from iron to uranium were made [5]. While light elements (Be and lighter) emerged from the Big Bang, fusion reactions in stars cannot produce elements heavier than iron. Heavier elements are thought to be produced during explosive events, such as type I supernovae via rapid neutron capture, the so-called r-process [6]. Since the neutron capture rate is generally much faster than the β-decay rate, successive neutron capture occurs and heavy nuclei are synthesized near the neutron drip line. Later, after the neutron flux has diminished, these exotic nuclei β-decay to the valley of stability. The r-process itself is dependent on details of nuclear structure, e.g., the location of the drip line, the existence of closed shells, β-decay lifetimes, etc. Consequently, a focus for nuclear physics research in the coming decades will be the very exotic nuclei approaching the neutron drip line. Thus, there are several proposals for experimental facilities dedicated to the study of exotic nuclei. At the same time, if these new experimental facilities are to realize thir full potential, substantial improvements in nuclear structure theory is needed.

In these lectures, I will discuss the latest developments in computational methods to arrive at a comprehensive and microscopic description of the structure of atomic nuclei. I will primarily focus on configuration interaction methods, which often provide the most detailed information available on the structure of nuclei. These lecture notes will be organized in the following manner. First, in Section 2 I will give a brief description of configuration interaction, or CI, methods. A description of the inter-nucleon interactions based effective field-theory is given in Section 3, while applications of the ab initio, No-core Shell Model will be described in Section 4. An alternative to matrix diagonalization methods, the Auxiliary-field Monte Carlo method, will be described in Section 5, while concluding remarks and the future prospects are outlined in Section 6.

2 Configuration interaction: The basics

The quantum many-body problem is the foundation of much of modern physics and chemistry, and one of the great challenges in theoretical physics is to develop a fully microscopic solution that includes the full range of quantum correlations. Configuration-interaction (CI) methods, such as the nuclear shell model, have been a traditional method of choice. Some excellent reference material describing shell-model methods an applications are found in Refs. [7,8]

The principal behind CI is a convenient basis that can serve as the foundation to construct the exact many-body wave function. For ab initio calculations for the lightest nuclei, say $A \leq 5$, an A-body harmonic oscillator basis in the Jacobi coordinates is very efficient [3]. It has the principal advantage that it includes only the intrinsic degrees of freedom, thus the basis dimension is quite small. In addition, it is rather straightforward to include Hamiltonians up to three-body clusters in fairly large model spaces. Indeed, calculations for $A = 3$ and $A = 4$ nuclei have been performed in model spaces containing 36 and 18 major oscillator shells, respectively. For $A \geq 5$ nuclei, severe computational problems arise in anti-symmetrizing the basis, and it is in fact currently not possible to go beyond four major oscillator shells for $A = 5$ and three major shells for $A \geq 6$ [3]. The principal alternative is the spherical three-dimensional harmonic oscillator, which we use to define a set single-particle states that the valence particles will occupy (actually any spherical basis, such as Woods-Saxon or Hartree-Fock can be used, although for ab initio calculations the harmonic oscillator has distinct advantages). The valence particles are then permitted to occupy these single-particle orbitals and influence each other through an effective interaction. In this valence space, is a set of N_D basis states, ϕ_i, that we can use

to construct the eigenstates of the Hamiltonian $\hat{H}$ i.e., $\Psi_\mu = \sum_i \alpha_{\mu i}\phi_i$. For convenience, these basis states are typically chosen to be product wave functions, or Slater determinants (SD), with well defined parity and z-component of angular momentum, J_z; the so-called M-scheme basis (although, sometimes wave functions with projected angular momentum, J, and isospin, T, are used). The utility of the M-scheme is that using second-quantization, the SDs may simply be represented on a computer as an integer word. Since the occupation of any single-particle state is either 0 or 1, we can associate each bit with a specific single-particle state and we can represent the following Slater determinant as 16-bit integer word

$$a_{10}^\dagger a_6^\dagger a_2^\dagger |0\rangle = 0000001000100010 = 2^{10-1} + 2^{6-1} + 2^{2-1} = 545. \tag{1}$$

Consequently, each SD is compactly stored in computer memory. Further, a full array of bit-manipulation routines exist that permit efficient operations on the set of SDs.

The number of basis states required for CI applications generally increases dramatically with particle number. A rough estimate of the basis dimension required for a CI calculation can be found from the total number of SDs in the basis, i.e., with all J_z, J, and T values, which is given by

$$N_D^{tot} \approx \begin{pmatrix} N_s^p \\ N_v^p \end{pmatrix} \begin{pmatrix} N_s^n \\ N_v^n \end{pmatrix}, \tag{2}$$

where $N_s^{p(n)}$ is the number of proton (neutron) single-particle states in the configuration space, and $N_v^{p(n)}$ is the number of proton (neutron) valence particles. In general, N_D^{tot} is roughly an order-of-magnitude greater than the number of states with the minimum value of J_z, which are sufficient to generate all the eigenstates of the system. In general, the numerical effort for Hamiltonians limited to just two-body interactions scales as $N_D^{1.25}$, while if three-body interactions are present the numerical effort scales as $N_D^{1.5}$. The main numerical challenge for CI is to develop efficient algorithms to extend the dimension to the largest available. Presently, the computational limits for two-body and three-body interactions interactions are for $N_D \approx 10^{9-10}$ and $N_D \approx 10^7$, respectively. It must be remarked that CI with matrix-diagonalization is essentially a brute-force method that will always face computational restrictions limiting the basis dimension. Consequently, other methods, such as the Auxiliary-field Monte Carlo method outlined in Section 5 need to be explored. On the other hand, matrix diagonalization is a powerful method that yields detailed information about individual states. Currently, powerful M-scheme shell-model programs such as ANTOINE (two-body only) [9], Many-Fermion Dynamics [10], and REDSTICK [11] exist on the market to perform a wide range of detailed nuclear structure studies for systems with large basis dimension. Here, a short description of the on-the-fly techniques used in codes such as ANTOINE and REDSTICK will be presented.

Mathematically, CI reduces to a matrix-diagonalization problem by finding the eigenvalues of the matrix $H_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle$. Since the basis dimension can be quite large and we are most often interested in only the lowest lying states, the traditional algorithm of choice to find the eigenvalues of the matrix $\mathbf{H}$ is the Lanczos algorithm. One starts with an arbitrary vector $\mathbf{v}_1$, apply the Hamiltonian matrix, yielding a second vector that may be decomposed in to two vectors: the original vector $\mathbf{v}_1$ and a second vector orthogonal $\mathbf{v}_2$. Applying, $\hat{H}$ to $\mathbf{v}_2$ we can proceed to transform $\mathbf{H}$ into tridiagonal form via

$$\begin{aligned}
\hat{H}\mathbf{v}_1 &= \alpha_1\mathbf{v}_1 + \beta_1\mathbf{v}_2 \\
\hat{H}\mathbf{v}_2 &= \beta_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \beta_2\mathbf{v}_3 \\
\hat{H}\mathbf{v}_3 &= \beta_2\mathbf{v}_2 + \alpha_3\mathbf{v}_3 + \beta_3\mathbf{v}_4 \\
\hat{H}\mathbf{v}_4 &= \beta_3\mathbf{v}_3 + \alpha_4\mathbf{v}_4 + \beta_4\mathbf{v}_5.
\end{aligned} \tag{3}$$

In the event of degenerate eigenvalues, the Lanczos process will terminate once all the space of n_d non-degenerate eigenvalues has been spanned with $\beta_{n_d-1} = 0$. While this is an inefficient algorithm to bring the whole matrix into tridiagonal form, it has the distinct advantage that if we truncate the procedure at $\mathbf{v}_n$ (the n^{th} iteration) the eigenvalues of the resulting tridiagonal matrix defined by the diagonal elements $(\alpha_1 ... \alpha_n)$ and the off-diagonal elements $(\beta_1 ... \beta_{n-1})$

converge to extreme eigenvalues of the full matrix **H**. As a consequence, one can generally obtain the lowest ten eigenvalues in 150-200 iterations regardless the dimension of **H**.

Computationally, the main question is now how to apply the Hamiltonian to the Lanczos vectors in the most efficient manner; particularly to exploit the many advantages of modern parallel architectures. In some ways, the most efficient procedure would be to pre-compute the Hamiltonian matrix. The difficultly with this approach, however, is that the matrix itself can be quite large and demand more memory than is available. Printing the matrix to disk and retrieving it when needed is an alternative, but in general, input/output (I/O) operations are quite slow, and thus severely limit the size of the problem that can be achieved. An alternative is the MFD code, where the entire matrix is distributed across many thousands of processors. Sometimes, however, the problem at hand is so large that will not fit into the number of processors available. In this case, on-the-fly methods, where we essentially recompute the matrix at each Lanczos iteration offer an excellent alternative. This concept was proposed with the code ANTOINE and then extended in REDSTICK to include three-body interactions as well as parallel platforms.

We start by an appropriate ordering of the basis states that will permit a fast look-up of the Lanczos vector once we have the indices of the proton and neutron states [9]. First, we separately construct the required proton and neutron SDs, and priority sort them first by parity, then $J_z^{P(N)}$, and finally oscillator quanta $\hbar\Omega^{P(N)}$ (if at some point we need to search through this list for a particular SD, it is useful to put the individual integer words within these blocks into ascending order). The full list of proton-neutron SDs can then made by first looping through the list of proton SDs and then looping through the appropriate list of neutron SDs with the constraint applied so that the full SD has the parity, J_z and $\hbar\Omega$ desired for the particular calculation. For illustrative purposes, consider the following set of proton and neutron SD's (each with positive parity and $0\hbar\Omega$) needed to construct a full proton-neutron basis with total $J_z = 0$,

$$\begin{array}{lll} J_z = -1 & |\phi_1^P\rangle, & |\phi_1^N\rangle \\ & |\phi_2^P\rangle, & |\phi_2^N\rangle \\ & |\phi_3^P\rangle, & \\ J_z = 0 & |\phi_4^P\rangle, & |\phi_3^N\rangle \\ & & |\phi_4^N\rangle \\ J_z = 1 & |\phi_5^P\rangle, & |\phi_5^N\rangle \\ & |\phi_6^P\rangle, & |\phi_6^N\rangle. \end{array} \tag{4}$$

The full list of the twelve combined SD's with the appropriate index may be constructed as

$$\begin{array}{l} 1 : |\phi_1^P\rangle, |\phi_5^N\rangle \\ 2 : |\phi_1^P\rangle, |\phi_6^N\rangle \\ 3 : |\phi_2^P\rangle, |\phi_5^N\rangle \\ 4 : |\phi_2^P\rangle, |\phi_6^N\rangle \\ 5 : |\phi_3^P\rangle, |\phi_5^N\rangle \\ 6 : |\phi_3^P\rangle, |\phi_6^N\rangle \\ 7 : |\phi_4^P\rangle, |\phi_3^N\rangle \\ 8 : |\phi_4^P\rangle, |\phi_4^N\rangle \\ 9 : |\phi_5^P\rangle, |\phi_1^N\rangle \\ 10 : |\phi_5^P\rangle, |\phi_2^N\rangle \\ 11 : |\phi_6^P\rangle, |\phi_1^N\rangle \\ 12 : |\phi_6^P\rangle, |\phi_2^N\rangle. \end{array} \tag{5}$$

Now, with each proton SD we store the starting position minus one in the full SD list, e.g., `pstart`(4)=6, and for each neutron SD, we store its relative position within its list, e.g., `nstart(4)`=2. Consequently, once we have the index for the proton (i_P) and neutron (j_N) SD, we can recover the index in the combined basis by simply adding the two integers

$$\texttt{index} = \texttt{pstart}(i_P) + \texttt{nstart}(j_N). \tag{6}$$

It is important to note that this ordering scheme removes the need to perform a search for the combined basis state, and is one of the fastest means to find the index of the full state. It also limits, somewhat, the type of restrictions that can be applied. For example, and truncation based on partition (the number of protons and neutrons in explicit orbits) is not possible. However, a truncation on oscillator quanta, $\hbar\Omega$, for the full state is. In this regard, we note that one is, of course, free to define the $\hbar\Omega$ values for each orbit, thus giving more flexibility in implementing truncations.

Regarding the application of the Hamiltonian to a given SD, $|\phi_i^P\rangle|\phi_j^N\rangle$, it is clear that if we store all the indices to the states $|\phi_{i'}^P\rangle|\phi_{j'}^N\rangle$ that are are connected by the Hamiltonian that this would essentially be equivalent to storing the full Hamiltonian matrix. Instead, we will focus on connections within the separate proton and neutron bases. We begin by noting that we may rewrite the proton-neutron (PN) component of the Hamiltonian as the product of two one-body operators,

$$H^{PN} = \sum_{(\alpha\beta)(\gamma\delta)} V^{PN}_{(\alpha\beta)(\gamma\delta)} \pi^\dagger_\alpha \pi_\beta \nu^\dagger_\gamma \nu_\delta, \tag{7}$$

where $\pi^\dagger$ and $\nu^\dagger$ denote proton and neutron creation operators, respectively. Then, for each proton (neutron) SD, we store the full list of states $|\phi_{i'}^{P(N)}\rangle$ that differ from the original state $|\phi_i^{P(N)}\rangle$ by a one-body jump. We then priority sort this list by the parity, $J_z^{P(N)}$, and $\hbar\Omega^{P(N)}$ of the final state $|\phi_{i'}^{P(N)}\rangle$. The action of the proton-neutron Hamiltonian is then accounted for by first looping over all the possible proton one-body jumps on the initial state $|\phi_i^P\rangle$ followed by a loop over the set of neutron one-body jumps on the initial state $|\phi_j^N\rangle$ so that the parity, J_z, and $\hbar\Omega$ of the final combined SD is permitted in the calculation (note that parity and J_z are conserved, while $\hbar\Omega$ typically is restricted within a range, e.g., $0 \leq \hbar\Omega \leq 4$). The information that needs to be stored is the index i' of the final state, the index of one-body operator $\pi^\dagger_\alpha \pi_\beta$, and the phase of the operation. These quantities can be compactly stored in a one-dimensional arrays. We note, however, that we also need to have a separate array pointing to starting positions in this array for the parity, J_z, and $\hbar\Omega$ for each initial state. Given that the number of elements in this array are not uniformly distributed, the most memory compact method is to use a derived type in FORTRAN 90. The power of "factorizing" the PN-Hamlitonian this way is that typically the number of one-body jumps in the separate proton and neutron spaces are not very large, and in most cases can easily fit into the memory of even modest computers. Also, while using this "factorization" method, we can see the utility of the ordering described in Eqs. (5) and (6), as in the loops we only know the initial and final proton and neutron SD indices, i, i' and j, j', respectively, and not the index of the combined SD.

In general, the application of proton-proton (PP) and neutron-neutron (NN) components of the Hamiltonian is simpler, and there are two options. The first, and probably most efficient, is to pre-compute the PP(NN)-Hamiltonian in the proton (neutron) SD space, noting that parity and $J_z^{P(N)}$ are conserved. In this case, one starts with the initial state i and stores the matrix elements of the PP-Hamiltonian and the index i' to the final states. This can easily be accomplished by compacting both quantities into vectors, with a separate integer array pointing to the starting position of the PP matrix for each state. To apply the Hamiltonian, we start with each initial state i and loop over all the final PP states. Then, we perform a loop over the appropriate final neutron states noting that it must be the same for the initial and final proton states. A similar procedure is performed for the NN-Hamiltonian.

In the event that memory is limited and the full PP and NN matrices can't be stored in resident memory, an alternative is to utilize the fact that any PP-matrix element may be written

as

$$\langle \phi_{i'}^P | H^{PP} | \phi_i^P \rangle = \sum_{\phi_k^{P-2}} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}^{PP} \langle \phi_{i'}^P | \pi_\alpha^\dagger \pi_\beta^\dagger | \phi_k^{P-2} \rangle \langle \phi_k^{P-2} | \pi_\gamma \pi_\delta | \phi_i^P \rangle, \tag{8}$$

where a complete sum of intermediate states $|\phi_k^{P-2}\rangle$ with two particles removed is inserted between the creation and annihilation operators. To use this method, for each intermediate state $|\phi_k^{P-2}\rangle$ one first makes the sorted list (on parity, J_z, and $\hbar\Omega$) of all states $|\phi_i^P\rangle$ that can be reached by adding two particles. To apply the Hamiltonian, we begin with a loop over the intermediate $P-2$ states, and then successively loop over the initial and final SDs $|\phi_i^P\rangle$ and $|\phi_{i'}^P\rangle$, respectively. Just as in the stored case, a loop over the common neutron SD is performed, giving the index of the initial and final combined SD.

As one might expect, the application of a three-body Hamiltonian is somewhat more complicated, but basically follows the same algorithm. Again, the proton-proton-neutron (PPN) and proton-neutron-neutron (PNN) components are the most difficult to work with. The most straightforward approach is to follow the same general algorithm as in the PN-Hamiltonian. Except now, a full list of states connected by two-body jump is needed. While this is the most straightforward approach, it does have the difficulty that the number of two-body jumps can be quite large. This is because, unlike the PP case, the parity and J_z of the initial and final states can be different. For large calculations, it would be necessary to split the number of two-body jumps across multiple processors. In general, this is fairly straight forward, as one can simply count the number of two-body jumps and divide the initial states, i, across the processors so that full range of two-body jumps is contained in resident memory. As will be discussed below, this division may also help with load-balancing on multiple processor systems. The two-body jump approach can face memory limitations, and in some cases it may not be possible to store all the jumps in resident memory. An alternative, which was the approach used in the first version of REDSTICK, but is most likely 4-8 times less efficient, is to use the set of intermediate $P-2$ states discussed above for the PP-Hamiltonian. Here, just as in the PP-Hamiltonian, we begin with a loop over the full set of intermediate $P-2$ states, then loop over the set of initial i and final i' proton SDs. Then, we loop over the initial neutron state and the set of one-body jumps to the final neutron state. Again, we note that the one-body jumps associated with the final neutron state are constrained so that the final combined SD has the appropriate parity, J_z, and $\hbar\Omega$.

An important computational issue regarding the utilization of a three-nucleon interaction for many-body systems is actually the three-body Hamiltonian itself. In particular, the number of matrix elements required to define the Hamiltonian increases dramatically with the number of oscillator shells. for example, a $6\hbar\Omega$ calculation for light p-shell nuclei, which includes 8 major oscillator shells, requires of the order 700M numbers (or 2.8 GB of memory) just to specify the Hamiltonian in the M-scheme, i.e., three-body states with well defined parity, J_z and T_z. Increasing the model space to $8\hbar\Omega$, or 12 major oscillator shells, would require of the order 20G numbers. Consequently, it is not likely that it will feasible in the near future to push ab initio calculations for p-shell nuclei to beyond $8\hbar\Omega$.

In order to fully exploit modern computer systems, it is necessary to design a shell-model program that fully utilizes parallel architectures. At this time, the best method is to use the Message Passing Interface, or MPI [12]. Here, one can divide the execution into separate, independent calculations, and use MPI to communicate information between the individual processors. Since the Hamiltonain must be applied to each combined SD, $|\phi_i^P\rangle|\phi_j^N\rangle$, the most straight forward approach to parallelize the code is to divide the work on the individual SDs across multiple processors. This will, of course, give an incomplete Lanczos vector on each processor that is just an intermediate component of the full Lancozs vector. The full Lanczos vector is just the sum on each processor, which we can get by making a call to the MPI subroutine `MPI_ALLREDUCE`. It should be noted that while at first glance this is a fairly straightforward procedure, in practice one has to work ensure proper load balance. Towards this end, the final algorithm needs to be constructed so that the overall work on each processor is equivalent. Only in this way can efficient scaling to a large number of processors be achieved.

Table 1. ^{3}H binding energy for three modern nucleon-nucleon interactions compared with experiment.

Potential	Binding Energy (MeV)
Av18	-7.62
N^{3}LO	-7.86
CD-Bonn	-8.00
Experiment	-8.48

3 The interaction between nucleons

The inter-nucleon interactions lie at the center of any microscopic description of nuclei. Quantum chromo-dynamics (QCD) is, of course, universally believed to the correct theory describing the intrinsic structure of hadrons and the strong interaction between them. In the near future, large-scale lattice QCD calculations will likely verify that our current model for QCD is sufficient to describe the overall behavior of the nucleon-nucleon interaction. QCD calculations on the lattice, however, are not a practical starting point to describe the properties of nuclei with more than two, or perhaps at most three, constituents. Towards this end, an effective potential, or interaction, between the constituents that "models" QCD and permits a description of nuclei with point-like nucleons is needed. Until recently, the most common approach was to utilize a purely empirical potential whose form is hypothesized with parameters fit to nucleon scattering data and the properties of the deuteron. Many examples of this approach have been implemented. Most recently are the Argonne AVn potentials [13] (here n denotes the number of parameters in the fit) and the Bonn potentials [14] based on meson exchange theory.

Once we have determined the two-body interaction from the two-nucleon sector, it then becomes quite apparent that the two-nucleon interaction alone is insufficient to describe even the simplest many-body system, namely the triton and ^{3}He. this is shown in Table 1 where the triton binding energy obtained from three nucleon-nucleon interactions (including an effective-field theory potential described below) are compare with experiment. All realistic two-nucleon interactions underpredict the binding energy of even $A = 3$ nuclei. Note that these three potentials are also somewhat in disagreement with each other. This is mostly due to the fact that while each potential does equally well reproducing the NN phase shifts, they have different off-shell behaviors, which leads to non-locality that affects the overall binding energy for $A \geq 3$ nuclei. Naturally, the two-nucleon sector can tell us nothing about the non-local , or off-shell, components of the interaction. Thus, potentials such as Av18 are purely local, while meson-exchange based potentials, such as CD-Bonn, have non-local components. The principal source of non-locality in the Bonn potentials is well understood from pion exchange, where the potential in momentum space is given by

$$V^{\pi NN}(\mathbf{k}', \mathbf{k}) = -\frac{g_\pi^2}{4M_N^2} \frac{(E' + M_N)(E + M_N)}{(\mathbf{k}' - \mathbf{k})^2 + m_\pi^2} \left(\frac{\sigma_1 \cdot \mathbf{k}'}{E' + M_N} - \frac{\sigma_2 \cdot \mathbf{k}}{E' + M_N} \right) \times \left(\frac{\sigma_2 \cdot \mathbf{k}'}{E' + M_N} - \frac{\sigma_1 \cdot \mathbf{k}}{E' + M_N} \right) \quad (9)$$

where $\mathbf{k}$ and $\mathbf{k}'$ denote the relative momentum of the initial and final two-nucleon states, respectively, E and E' their relative energy, σ_i is the spinor of the i^{th} nucleon, M_N and m_π are the nucleon and pion mass, and g_π is the pion-nucleon coupling constant. The fact that two-nucleon interactions fail to bind even $A = 3$ nuclei suggests the presence of a three-nucleon interaction. In addition, the lack of uniqueness also suggests that the three-nucleon interaction is dependent on our choice of the NN-interaction. In this regard, various potentials were proposed, mostly based on two-pion exchange. Examples of these are the Illinois-2 [15] and Tucson-Melbourne potentials [16]. The obvious weaknesses to this approach is that it lacks the fundamental basis provided by QCD and there is little or no connection between the two- and three-body sectors.

An alternative mechanism to the inter-nucleon interactions is based on ideas introduced by Weinberg [17], which have come to be known chiral effective field theory (χEFT) [18]. χEFT

Fig. 1. Schematic view of the χEFT potential in terms of Feynman diagrams at the leading orders, i.e., Q^4 $\rightarrow$ N^{3}LO. The quantities C_D and C_E are the only new parameters required to fully define the three-body interaction up to order N^{3}LO.

is based on QCD through chiral perturbation theory and provides an elegant framework for mapping out the leading degrees of freedom in the nuclear Hamiltonian. Chiral symmetry imposes constraints on the possible momentum and spin dependencies in the nuclear forces. In addition, a momentum cutoff is introduced leading to a natural power counting scheme that limits the number of interaction terms in the nuclear Hamiltonian. With χEFT, one derives the nuclear forces up to a given order, manifestly including all the relevant QCD degrees of freedom to that order. χEFT potentials are often defined by the order in the expansion, e.g., leading order, next-to-leading order (NLO), next-to-next-to-leading order (N^{2}LO), etc. This is schematically illustrated [19] in Figure 1, where the Feynman diagrams at each order are represented for the two-body, three-body, and even four-body interaction. Note that the three-body interaction enters at N^{2}LO, while a four-body interaction first appears at N^{3}LO.

It is important to note that χEFT potentials are not completely devoid of empericism either, but rather give a framework for expanding and quantifying the nuclear Hamiltonian. Consequently, at each order, a set of parameters define the strength of each term in the Hamiltonian. While these parameters can in principle be computed with lattice QCD, they are generally determined by experimental data. Presently, an excellent description [19] of the nucleon-nucleon interaction has been obtained at N^{3}LO. This is illustrated in Figure 2 where the phase shifts for nucleon-nucleon scattering are displayed for χEFT potentials for NLO, N^{2}LO, and N^{3}LO.

Fig. 2. Nucleon-nucleon phase shifts for χEFT potentials; NLO (dotted line), N^{2}LO (dashed line), and N^{3}LO, (solid line). (from Ref. [19])

In regards to the three-nucleon interaction, only two new parameters (in addition to those fixed in the two-nucleon sector) are introduced. These are associated with the two contact terms (two lower diagrams) at N^{2}LO shown in Figure 1. These parameters are denoted C_D and C_E for the pion-plus-two-nucleon contact (left diagram) and three-nucleon contact (right diagram) terms, respectively. Currently, the explicit forms for the three-nucleon diagrams have only been derived at the order N^{2}LO. Consequently, in what follows (which is reported in detail in Ref. [20]), a study of the properties of the three-nucleon interaction will be performed considering the three-nucleon interaction at order N^{2}LO, and the two-nucleon interaction at order N^{3}LO. A fully consistent picture will require that all the two-, three-, and four-body terms be included at order N^{3}LO, which is underway. We note, however, that no new parameters are introduced at N^{3}LO, where the strengths of all the new diagrams are determined by the two-nucleon coupling constants. This is also true for the weaker four-body interaction that enters at N^{3}LO. All that would remain would be to redetermine the parameters C_D and C_E.

Fig. 3. Correlated values for the parameters C_D and C_E reproducing the $A = 3$ binding energies (dashed-dot:^{3}H, dashed-dot-dot: ^{3}He, solid: average of ^{3}H and ^{3}He). In the insets (a) and (b) are the ^{4}He binding energy and rms radius as a function of C_D (with C_E given by the solid line). The dashed lines in the insets represent the ^{4}He experimental data. (from Ref. [20])

Shown in Figure 3 are the values of C_D and C_E required to reproduce the binding energies of the $A = 3$ systems. The dashed-dot line represents ^{3}H, the dashed-dot-dot line, ^{3}He, and the solid line the averaged ^{3}H and ^{3}He binding energies. Note that C_D and C_E span a parabola,

and are not constrained by the $A = 3$ binding energies to a single value. In the insets (a) and (b), the ^{4}He binding energy and rms radius are shown, respectively, as a function of C_D in comparison to their corresponding experimental values (here, C_E was constrained to reproduce the averaged $A = 3$ binding energy). We note that across the range of C_D values the ^{4}He binding energy is essentially reproduced at the level of 200 keV. Given that this is roughly the accuracy that we can expect for the N^{2}LO diagrams, it is not possible to explicitly exclude larger values of C_D. There is a hint, however, from inset (b) that at larger C_D values the rms radius is increasing outside the physically acceptable range. This is also apparent in the $A = 3$ figure, where at larger C_D values the ^{3}H and ^{3}He curves diverge. This is in fact due to a larger radius, which affects the Coulomb energy. Combined with studies for heavier p-shell nuclei (to be described in the next section), at present we determine that the best overall description of the N^{2}LO three-body interaction is for $-1 \leq C_D \leq 0$.

The overall importance of the three-nucleon interaction will also be apparent in the next section, where calculations for p-shell nuclei will be shown. In addition to the very important effect of increasing the overall binding energy, the three-nucleon interaction also affects the structure of low-lying levels. In particular, the three-nucleon interaction is seen to have strong spin-orbit components, and may in fact be responsible for most of the spin-orbit physics exhibited in nuclei.

4 Ab initio calculations

With a description of the nucleon-nucleon and three-nucleon interactions at hand, we may proceed with a first-principle solution for systems with more than four particles. Several approaches can be utilized, with each having some specific advantages over the other. The three in use today are Green's Function Monte Carlo (GFMC), coupled clusters, and the no-core shell model (NCSM). Priamrily, we will focus on the NCSM in these lectures, but a quick description of the other two methods is in order.

The Green's function Monte Carlo method [1], whose starting point is in fact rather similar to the Auxiliary-field method described in Section 5 (except that it is carried out in coordinate space rather than Fock space), is based on the fact that the ground-state expectation value of any operator may be evluated from

$$\langle \hat{\Omega} \rangle_{GS} = \lim_{\beta \to \infty} \frac{\langle \phi_0 | \hat{\Omega} e^{-\beta \hat{H}} | \phi_0 \rangle}{\langle \phi_0 | e^{-\beta \hat{H}} | \phi_0 \rangle} \, , \tag{10}$$

where ϕ_0 is an arbitrary wave function not orthogonal to the exact ground state. In practice, however, the quality of the trial wave function does affect the convergence of the method. Generally, ϕ_0 is taken to be a variational wave function with with fairly simple configurations and short-range correlations put in via a Jastrow function. In addition, symmetries such as angular momentum are often built in. The Hamiltonian contains the kinetic energy as well as the two- and three-body potential in coordinate space and the integral is sampled with Monte Carlo methods. At present high quality results, which often can be thought of as a "gold-standard" for ab initio methods have been obtained for nuclei up to ^{12}C. Unfortunately, computational difficulties will limit the GFMC method to $A = 12$ for the near future. In addition, the GFMC method is limited to only potentials that are local in coordinate space, and thus cannot be utilized for the χEFT potentials described in Section 4.

Second are coupled cluster techniques [21], which while they are not limited in the form of the interaction, are generally best suited for systems with a closed shell, such as ^{16}O or ^{40}Ca. In coupled-cluster theory, one uses the correlated state $|\psi\rangle$ that is given by a correlation operator $\exp(\hat{T})$ acting on a single-particle product state $|\phi\rangle = \prod_{i=1}^{A} a_i^\dagger |0\rangle$ by

$$|\psi\rangle = e^{\hat{T}} |\phi\rangle. \tag{11}$$

The cluster operator $\hat{T}$ is given as a sum of one-, two-, up to A-particle cluster operators, namely

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots + \hat{T}_A, \tag{12}$$

where $\hat{T}_1$, $\hat{T}_2$, etc. are given by

$$\hat{T}_1 = \sum_{ia} t_i^a a_a^\dagger a_i,$$
$$\hat{T}_2 = \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i, \tag{13}$$

where the sums ij and ab run over occupied and unoccupied single-particle states in $|\phi\rangle$, respectively. At a given truncation in $\hat{T}_n$, one then minimizes the energy with respect to the quantities t_i^a, t_{ij}^{ab}, etc., leading to a set of complicated coupled equations. The power of coupled-cluster methods is that they are size-extensive, meaning that accurate results can be obtained for extraordinarily large systems with a relatively small limit on the cluster number. Indeed, reasonably accurate results are obtained with just $\hat{T}_1$ and $\hat{T}_2$, or singles and doubles, hence the moniker CCSD. Improved accuracy comes with triples (T), although in general this computationally more expensive, and often the full effect of the triples is approximated. Currently, studies have been performed for light nuclei, principally ^{4}He, including three-nucleon interactions [22].

4.1 The No-core Shell Model

The method utilized and described in these lectures is the no-core shell model (NCSM). The basic task at hand is to obtain solutions to the standard eigenvalue problem

$$(\hat{H} - E_\nu)|\Psi_\nu\rangle = 0, \tag{14}$$

where E_ν is the desired eigenvalue, $\hat{H}$ is the Hamiltonian, and Ψ_ν is the eigenfunction. The Hamiltonian is a key ingredient as it describes the kinetic motion of the constituent particles and their interaction with one another. Here, we consider a first-principles Hamiltonian consisting of the kinetic energy as well two- and three-body interactions

$$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}. \tag{15}$$

To Eq. (15) we add an oscillator potential in center-of-mass coordinate (which will later be subtracted, and thus has no effect on the full calculation)

$$\hat{H}_{COM} = \frac{Am}{2}\Omega^2 \mathbf{R}^2 = \frac{m\Omega}{2}\sum_i \mathbf{r}_i^2 - \frac{m\Omega^2}{2A}\sum_{i<j}(\mathbf{r}_i - \mathbf{r}_j)^2, \tag{16}$$

where Ω is the oscillator parameter, which essentially defines the size of the system. Collecting the one-body oscillator term with the kinetic energy, we then have a single-particle oscillator basis to construct our many-body Slater determinants,

$$\hat{H} = \sum_i \left(\frac{\hat{p}_i^2}{2m} + \frac{m\Omega}{2}\mathbf{r}_i^2\right) + \sum_{i<j}\left(V_{ij} - \frac{m\Omega^2}{2A}(\mathbf{r}_i - \mathbf{r}_j)^2\right) + \sum_{i<j<k} V_{ijk}. \tag{17}$$

The principal advantage of the oscillator basis is that it is the only convenient basis where the intrinsic and center-of-mass motion can separated exactly. This is easily achieved if the model space included in the calculation is complete up to a given number of $N_{\max}$ excitations in the oscillator (generally denoted as $N_{\max}\hbar\Omega$). On the other hand, the main weakness of the oscillator basis is that the single-particle wave functions defining the basis have the wrong asymptotic behavior. In general, because of the finite binding of the system, we would expect the bound single-particle wave functions to have an exponentially decaying behavior, whereas the asymptotic behavior of the oscillator wave functions is Gaussian in nature.

The principal difficulty with using CI methods to solve Eq. (30) is that in ab initio applications, short-range correlations in the inter-nucleon interaction require a large model space in order to achieve convergence. Indeed, even for the softer χEFT two-body potentials, excitations of up to at least $16\hbar\Omega$ are required in order to get converged ^{4}He results with the bare interaction. This many excitations for a nucleus such as ^{12}C would easily lead to a basis dimension in excess of 10^{15}, which for all intents and purposes is infinite.

This infinite basis problem can, in principle, be circumvented by the use of effective-interaction theory. First, one chooses a manageable subset of the original basis states leading to the slightly different eigenvalue problem

$$(\hat{H}_{\mathit{eff}} - E_\nu)\hat{P}|\Psi_\nu\rangle = 0, \tag{18}$$

where $\hat{P}$ is an operator that projects the exact solution Ψ_ν onto the chosen model space, E_ν is again the eigenvalue, and $\hat{H}_{\mathit{eff}}$ is an effective Hamiltonian that yields the *exact* solution of Eq. (30). Here, we chose the P-space to be defined by the number of $N_{\max}$ oscillator quanta in the many-body space. One derivation of $\hat{H}_{\mathit{eff}}$ is given by the famous Bloch-Horowitz equation [23],

$$\hat{H}_{\mathit{eff}} = \hat{H} + \hat{P}\hat{H}\frac{1}{E_\nu - \hat{Q}\hat{H}}\hat{Q}\hat{H}, \tag{19}$$

where $\hat{Q}$ is an operator that projects onto the portion of the shell-model space that is excluded in the calculation. The principal difficulty with the $\hat{H}_{\mathit{eff}}$ defined by Eq. (19) is that effective interaction itself depends on the solution E_ν. Thus, each eigenvalue has a different effective interaction and must be solved for self-consistently. In addition, Eq. (19) is the basis for the two-body effective interaction known as the G-matrix (e.g., see p. 339 of Ref. [7]).

4.2 Okubo-Lee-Suzuki Transformation

A more practical derivation of the effective interaction is to due to Okubo [24] and Lee and Suzuki [25]. Our task is to find a unitary transformation $e^{\hat{S}}$ so that

$$\hat{H}_{\mathit{eff}} = e^{-\hat{S}}\hat{H}e^{\hat{S}} \tag{20}$$

and the P- and Q-spaces are decoupled. The derivation begins with the eigenvalue equation

$$\begin{aligned}
&\hat{H}|\Psi_\nu\rangle = E_\nu|\Psi_n u\rangle \\
&e^{\hat{S}}e^{-\hat{S}}\hat{H}e^{\hat{S}}e^{-\hat{S}}|\Psi_\nu\rangle = E_\nu|\Psi_n u\rangle \\
&(\hat{P}+\hat{Q})e^{-\hat{S}}\hat{H}e^{\hat{S}}(\hat{P}+\hat{Q})e^{-\hat{S}}|\Psi_\nu\rangle = E_\nu(\hat{P}+\hat{Q})e^{-\hat{S}}|\Psi_\nu\rangle.
\end{aligned} \tag{21}$$

Requiring that $\hat{P}e^{-\hat{S}}\hat{H}e^{\hat{S}}\hat{Q} = \hat{Q}e^{-\hat{S}}\hat{H}e^{\hat{S}}\hat{P}$, we arrive at

$$\begin{aligned}
&\hat{P}e^{-\hat{S}}\hat{H}e^{\hat{S}}\hat{P}e^{\hat{S}}|\Psi_\nu\rangle = E_\nu\hat{P}e^{-\hat{S}}|\Psi_\nu\rangle \\
&\hat{H}_{\mathit{eff}}|\phi_\nu\rangle = E_\nu|\phi_\nu\rangle,
\end{aligned} \tag{22}$$

with $|\phi_\nu\rangle = \hat{P}e^{-\hat{S}}|\Psi_\nu\rangle$. Note that both $|\Psi_\nu\rangle$ and $|\phi_\nu\rangle$ are normalized to unity.

To determine the operator $\hat{S}$, we introduce the similarity transformation $e^{\hat{\omega}}$ so that $\hat{\omega} = \hat{Q}\hat{\omega}\hat{P}$, which leads to

$$\begin{aligned}
&\hat{\omega}^2 = 0 \\
&e^{\hat{\omega}} = 1 + \hat{\omega}.
\end{aligned} \tag{23}$$

Requiring that $\hat{\omega}$ decouples the Q-space from the P-space, namely that

$$\hat{Q}e^{-\hat{\omega}}e^{\hat{\omega}}\hat{P} = 0, \tag{24}$$

we find $e^{\hat{S}}$ given by

$$e^{\hat{S}} = (1 + \hat{\omega} - \omega^{\dagger})(1 + \hat{\omega}^{\dagger}\hat{\omega} + \hat{\omega}\hat{\omega}^{\dagger})^{-1/2}, \tag{25}$$

or

$$\hat{S} = \text{arctanh}(\hat{\omega} - \hat{\omega}^{\dagger}). \tag{26}$$

The hermitian effective Hamiltonian can now be defined in terms of the operator $\hat{\omega}$ as

$$\hat{H}_{\mathit{eff}} = (1 + \hat{\omega}^{\dagger}\hat{\omega})^{-1/2}(1 + \hat{\omega}^{\dagger})\hat{H}(1 + \hat{\omega})(1 + \hat{\omega}^{\dagger}\hat{\omega})^{-1/2}. \tag{27}$$

A couple of other observations are in order. First, in order to achieve the exact decoupling in Eq. (24), $\hat{\omega}$ must be an A-body operator and cannot in general be approximated by an operator at a smaller cluster number. Second, the product operator $\hat{\omega}^{\dagger}\hat{\omega}$ acts solely within the P-space and has an implicit sum over the complete set intermediate Q-space states. Likewise $\hat{\omega}\hat{\omega}^{\dagger}$ acts only in the Q-space. Finally, it is clear that in principle $\hat{H}_{\mathit{eff}}$ now contains two-, three-, and up to A-body components even if the original interaction is only two-body in nature. The overall importance of the many elements of $\hat{H}_{\mathit{eff}}$ are evident. First, the renormalization accounts short-range correlations caused by the short-range repulsion of the bare interaction. Second, the higher-body terms account for the truncation to the P-space. As a consequence, the relative importance of the higher-body terms diminishes as the P-space increases. Finally, it is also important to realize that the Okubo-Lee-Suzuki procedure does not lead to an effective Hamiltonian that is variational. As a consequence, convergence may be achieved from either above or below the exact solution.

Two useful quantities that we can extract once we have solved for the P-space eigenvalues $|\phi_{\nu}\rangle$ are the measure of the exact wave function $|\Psi_{\nu}\rangle$ lying within either the P- or Q-space:

$$\begin{aligned}
\langle\Psi_{\nu}|\hat{P}|\Psi_{\nu}\rangle &= \langle\phi_{\nu}|e^{-\hat{S}}\hat{P}e^{\hat{S}}|\phi_{\nu}\rangle = \langle\phi_{\nu}|(1 + \hat{\omega}^{\dagger}\hat{\omega})^{-1}|\phi_{\nu}\rangle \\
\langle\Psi_{\nu}|\hat{Q}|\Psi_{\nu}\rangle &= \langle\phi_{\nu}|e^{-\hat{S}}\hat{Q}e^{\hat{S}}|\phi_{\nu}\rangle = \langle\phi_{\nu}|(1 + \hat{\omega}^{\dagger}\hat{\omega})^{-1/2}\hat{\omega}^{\dagger}\hat{\omega}(1 + \hat{\omega}^{\dagger}\hat{\omega})^{-1/2}|\phi_{\nu}\rangle.
\end{aligned} \tag{28}$$

4.3 Solution for $\hat{\omega}$

In this section, we give a formal solution for the operator $\hat{\omega}$. We note that a full representation for $\hat{\omega}$ actually requires for the full wave function $|\Psi_{\nu}\rangle$, which is obviously not practical in general. However, the solution outlined here is the basis for the ansatz used to define the effective interaction used in the No-core Shell Model. In addition, there are situations where one wishes to project a full solution onto a smaller space, thereby giving an effective interaction in the smaller space that exactly reproduces the eigenvalues in a larger model space.

We begin by denoting the many-body basis states $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ that define the P- and Q-spaces, respectively. In addition, we note that there are exactly N_{α_P} states $|\alpha_P\rangle$ within the P-space. We can write $\hat{\omega}$ as

$$\hat{\omega} = \sum_{\alpha_P\alpha_Q} \langle\alpha_Q|\hat{\omega}|\alpha_P\rangle|\alpha_Q\rangle\langle\alpha_P| \tag{29}$$

and the Hamiltonian as

$$\hat{H} = \sum_k E_k|k\rangle\langle k|, \tag{30}$$

where the states $|k\rangle$ are the eigenstates of the full Hamiltonian. Using the definitions of Eqs. (29) and (30) and the decoupling condition of Eq. (24), we have for any Q-space state

$$\langle\alpha_Q|k\rangle = \sum_{\alpha_P}\langle\alpha_Q|\hat{\omega}|\alpha_P\rangle\langle\alpha_P|k\rangle. \tag{31}$$

Inverting this equation, we have for the matrix elements of $\hat{\omega}$

$$\langle \alpha_Q | \hat{\omega} | \alpha_P \rangle = \sum_k^{N_{\alpha_P}} \langle \alpha_Q | k \rangle \langle \tilde{k} | \alpha_P \rangle, \tag{32}$$

where the sum runs over only N_{α_P} exact eigenvalues $|k\rangle$ of $\hat{H}$, and $\langle \tilde{k} | \alpha_P \rangle$ denotes the inverse of the symmetric $N_{\alpha_P} \times N_{\alpha_P}$ matrix $\langle \alpha_P | k \rangle$.

With the matrix elements of $\hat{\omega}$ defined in Eq. (32), we can proceed to compute an effective interaction from Eq. (27) that will exactly reproduce the full space eigenvalues. Further, using the norms defined in Eq. (28) we can also compute the expectation value for any operator.

4.4 The effective interaction within the No-core Shell Model

As was mentioned in the previous section, the formal solution for the $\hat{\omega}$ operator is in actuality impractical for realistic calculations because it actually requires the full-space solutions. Instead, the No-core Shell Model relies on the ansatz that an effective interaction can be derived by solving the Okubo-Lee-Suzuki procedure at a particular cluster level. Overall, the procedure outlined here is guaranteed to converge as the size of the P-space increases (as the effective interaction will converge to the bare interaction) or as the size of the cluster approximation in the effective interaction increases.

To derive an n-body effective interaction, we first set up the Hamiltonian as defined in Eq. (17) for the system of interest (i.e., a specific A value) and define the P- and Q-space for the A-body system. We then let the n-body states $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ denote the states required to specify the n-body Hamiltonian matrix elements for the many-body calculation. In this case, there are now d_P states $|\alpha_P\rangle$. The effective interaction for the A-body NCSM calculation now requires that we obtain d_P eigenvalues, $|k\rangle$ of the n-body Hamiltonian matrix $\langle \alpha' | \hat{H} | \alpha \rangle$. The n-body interaction is now defined by the P-space n-body matrix elements

$$\langle \alpha'_P | \hat{H}_{\mathit{eff}} | \alpha_P \rangle = \langle \alpha'_P | (1 + \hat{\omega}^\dagger \hat{\omega})^{-1/2} (1 + \hat{\omega}^\dagger) \hat{H} (1 + \hat{\omega}) (1 + \hat{\omega}^\dagger \hat{\omega})^{-1/2} | \alpha_P \rangle, \tag{33}$$

where the n-body matrix of $\hat{\omega}$ are given by Eq. (32).

caption^{4}He binding energy with the χEFT Idaho-A potential as a function of model space size.

4.5 Results of NCSM calculations with two-body interactions

In this section, the results of several NCSM calculations utilizing two-nucleon interactions will be shown. First, as an overall demonstration of the power of the effective interactions derived with the Okubo-Lee-Suzuki method, in Figure 4 we show a calculation for the ^{4}He binding energy with the two-body χEFT Idaho-A potential as a function of the model space size $N_{\max}$ for the bare two-body interaction (circle : dotted line), two-body effective (up triangle : dashed), three-body effective (down triangle : solid), and four-body effective (cross : dashed-dot-dot). As mentioned in Section 3, the χEFT potentials tend to be soft, and convergence for the bare interaction is achievable for $N_{\max} \approx 16$. We note that for potentials with substantially harder cores, such as the Argonne Avn potentials, one would need $N_{\max} \geq 50$ to achieve similar convergence with the bare potential. From the figure, one sees that the effective interaction substantially improves the result even for the two-body clusters at $N_{\max} = 6$. On the other hand, the three-body effective interaction shows significant stability and near convergence for $N_{\max} \geq 4$.

Fig. 4. ^{6}Li binding energy with the χEFT N^{3}LO potential as a function of oscillator parameter and model space size for the bare potential and the two-body effective interaction.

In Figure 5 the results [26] of an NCSM calculation for ^{6}Li binding energy are shown as a function of the oscillator parameter $\hbar\Omega$ as well as the model space size $N_{\max}$. The solid lines are calculations for the two-body effective interaction while the dot and dashed lines are the results obtained with the bare potential. This behavior of the binding energy in Figure 5 is characteristic of NCSM calculations for $A \geq 5$, where the binding energy tends to span a parabola as a function of the oscillator parameter. Overall, the two-body effective interaction shows convergence in the binding energy at $\sim$ -29.5 MeV (less change in the absolute value with increasing $N_{\max}$). In addition, as the size of the model space increases the dependence on the oscillator parameter tends to lessen (decreasing curvature).

Fig. 5. Low-lying spectrum obtained for ^{10}B with the two-nucleon CD-Bonn potential as a function of model space (denoted by the $N_{\max}\hbar\Omega$ value under each spectrum column) compared with experiment.

In addition to substantially underbinding atomic nuclei, the nucleon-nucleon interaction is also inadequate for describing the low-lying structure of some nuclei. While the ordering of low-lying states is roughly in agreement with experiment for $A \leq 9$, the situation is very different for the odd-odd nucleus ^{10}B (as well as $A = 11$ and 13 nuclei). Shown in Figure 6 is the spectrum obtained for ^{10}B with the CD-Bonn potential as a function of model space (denoted by $N_{\max}\hbar\Omega$ along the bottom of the figure) in comparison with experiment. One sees that while the excitation energy of the $J = 3^+$ state is decreasing with larger $N_{\max}$, the $J = 1^+$ state is predicted to be the ground state. This feature is common to ALL realistic two-nucleon interactions. This behavior, along with the fact that NN-interactions substantially underbinding nuclei, points to a deficiency in the two-nucleon interaction itself and the need for a three-nucleon interaction.

Fig. 6. Low-lying spectrum obtained for ^{10}B the χEFT potentials as a function of the parameter C_D.

4.6 Results of NCSM calculations with three-body interactions

In this section, the effects of the three-nucleon interaction on nuclear structure will be demonstrated. Previously, GFMC calculations were performed with the empirical Illinois-2 potential, where parameters were fit to the energies of p-shell nuclei [15]. In the No-core Shell Model, the first studies were with three-nucleon interactions [27] were the Tucson-Melbourne three-nucleon interaction [16]. Here, I will focus on the results of a recent study using χEFT potentials [20]. In the NN sector, the N^{3}LO interaction was used, while the χEFT three-nucleon interaction at N^{2}LO described in Section 3 was added to it. As mentioned before, the two parameters C_D and C_E are not well determined from just the $A = 3$ binding energies, so an important part of the study was to ascertain how the structure of nuclear states evolve with the parameters. Shown in Figure 7 the spectrum of the low-lying levels in ^{10}B is shown with different values of the parameter C_D (the C_E parameter was constrained by to reproduce the $A = 3$ binding energy as shown in Figure 3). The most important feature is that in all cases the ordering of the $J = 3^+$ and $J = 1^+$ is correct. This is principally due to the fact that the two-pion exchange terms in the three-nucleon interaction contribute strongly to the effective spin-orbit interaction. Unfortunately, the ^{10}B spectrum alone does not constrain the C_D parameter. Overall, reasonable agreement with the experimental spectrum is certainly achieved in the range $-1 \leq C_D \leq +1$. Also, for the model space defined by $N_{\max} = 6$ and $C_D = -1$, the computed binding energy

is -64.03 MeV, which is in much better agreement with the experimental value of $-64.7507(3)$ MeV than with the NN-interaction alone. Thus, the three-nucleon interaction provides both more binding energy and important spin-oribit interactions.

Fig. 7. Dependence on the C_D with C_E constrained by the $A = 3$ binding energy fit for different basis sizes for: ^{6}Li quadrupole moment, ^{10}B B$(E2; 3^+_1 0 \rightarrow 1^+_1 0)$/B$(E2; 3^+_1 0 \rightarrow 1^+_2 0)$ ratio, and the ^{12}C B$(M1; 0^+0 \rightarrow 1^+1)$. The HO frequency of $\hbar\Omega$= 13, 14, 15 MeV was employed for ^{6}Li, ^{10}B, ^{12}C, respectively. In the inset of the ^{12}C figure, the convergence of the B$(M1; 0^+0 \rightarrow 1^+1)$ is presented for calculations with (using $C_D = -1$) and without the NNN interaction.

The influence of the three-nucleon interaction on spin-orbit properties is also illustrated in Figure 8, where several structure quantities are plotted for different model space sizes as a function of the parameter C_D (with the parameter C_E fixed by the $A = 3$ binding energy). In the upper panel is the ground-state quadrupole moment, while the middle panel shows the ratio of the B$(E2)$ value for the transition in ^{10}B from the first $J = 3^+$, $T = 0$ state (3^+0) to the first and second $J = 1^+$, $T = 0$ states. The bottom panel is the B$(M1)$ value for the transition between the $J = 0^+$, $T = 0$ ground state and the first $J = 1^+$, $T = 1$ state. In each panel the experimental value is denoted by the dashed line. In general, we find a trend towards convergence for each quantity with increasing $N_{\max}$. In addition, overll better agreement is achieved for each quantity (as well as the ^{10}B spectrum) for $C_D \approx -1$. Lastly, the inset in the bottom panel shows the convergence of the ^{12}C B$(M1)$ value with $(C_D = -1)$ and without the three-nucleon interaction. Here, substantially better agreement with experiment is achieved while including the three-nucleon interaction. Indeed, this result strongly illustrates the "spin-orbit" character of the three-nucleon interaction. This quantity is very sensitive to the breaking of SU(4) symmetry [28], as this is a transition between two different SU(4) irreps, which in the limit that SU(4) is a good symmetry would be forbidden, as is indicated by the small value for the NN-interaciton alone. On the other hand, spin-orbit interactions break SU(4) symmetry, which leads to a larger transition amplitude.

In the past couple of years substantial progress towards a first principles understanding of the structure of nuclei has been made. Indeed, many efforts underway now have progressed to point that a careful study of the properties of the three-nucleon interaction is now possible. Towards this end, large basis CI calculations for many-body systems are indispensable. They offer signatures not available in the three- and four-nucleon systems. Indeed, we are now coming to the somewhat surprising conclusion that the three-nucleon interaction is very much responsible for what we have come to know as the "spin-orbit" properties in nuclei. As such, they are very much responsible for the magnitude of Gamow-Teller transitions in nuclei. With these successes in mind, however, we still need to remember that thus far the three-nucleon interaction terms were derived at order N^{2}LO, while the two-nucleon interaction was determined at N^{3}LO. Thus, it is important that a fully consistent study of the inter-nucleon interactions be carried out at N^{3}LO (note that this would also include a small four-body interaction).

5 Auxiliary Field Monte Carlo methods

As mentioned in Section 2, the CI basis dimension increases dramatically with particle number. If we consider a model space with $N_s^{p(n)} \sim 40$ and $N_v^{p(n)} \sim 20$, which would be typical for $A \sim 90$ nuclei, the matrix dimension would be of the order 10^{20}. Given that the computational effort scales as $N_D^{1.25}$ and current limits are of the order 10^{10}, we would require a computer 10^{12} times more powerful than any available today. Monte Carlo methods offer an attractive alternative to CI as their computational effort scales more gently with particle number. Indeed, Monte Carlo methods have been applied to a wide variety of many-fermion problems in physics and chemistry; with applications in condensed matter, nuclear structure, and lattice quantum chromodynamics (see Ref. [29]). Unfortunately, Monte Carlo methods applied to fermionic systems generally suffer from the well-known sign problem (where the sampling weight function

is not positive definite), which substantially limits their efficacy. Here, we will address the sign problem with the Auxiliary-Field Monte Carlo (AFMC) method [30] based on the Hubbard-Stratonovich (HS) transformation [31].

The AFMC method for generic rotationally Hamiltonians is outlined in detail in Ref. [32], and here we present the central features germane to our solution to the sign problem. AFMC is based on the imaginary-time evolution operator $e^{-\beta\hat{H}}$ to either filter from an arbitrary trial wave function, ϕ_0, the ground-state (GS) value for the operator $\hat{\Omega}$ via

$$\langle\hat{\Omega}\rangle_{GS} = \lim_{\beta\to\infty} \frac{\langle\phi_0|e^{-\beta\hat{H}/2}\hat{\Omega}e^{-\beta\hat{H}/2}|\phi_0\rangle}{\langle\phi_0|e^{-\beta\hat{H}}|\phi_0\rangle} \,, \tag{34}$$

or to compute the thermal expectation value $\langle\hat{\Omega}\rangle_\beta$

$$\langle\hat{\Omega}\rangle_\beta = \mathrm{Tr}_{(Z,N)}\left[e^{-\beta\hat{H}}\hat{\Omega}\right] / \mathrm{Tr}_{(Z,N)}\left[e^{-\beta\hat{H}}\right] \,, \tag{35}$$

where $\mathrm{Tr}_{(Z,N)}$ denotes the Z-proton and N-neutron projected trace. Eqs. (34) and (35) are distinct and complementary approaches. Along with GS properties, the thermal formalism permits us to calculate structure information, such as electro-weak transition strengths, at finite temperature and is the optimal procedure for computing the density of states [**?**]. On the other hand, the "zero-temperature" formalism, Eq. (34), is an efficient way to compute GS observables.

Since any two-body Hamiltonian may be written in quadratic form as

$$\hat{H} = \sum_\alpha \varepsilon_\alpha\hat{\Theta}_\alpha + \frac{1}{2}\sum_\alpha V_\alpha\hat{\Theta}_\alpha^2 \,, \tag{36}$$

where here we choose $\hat{\Theta}_\alpha$ to be a generalized one-body density operator, V_α the strength of the two-body interaction, and ε_α the single-particle energies, we simplify $\exp(-\beta\hat{H})$ making use of the (HS) transformation [31]

$$e^{\frac{1}{2}\Lambda\hat{\Theta}^2} = \sqrt{\frac{|\Lambda|}{2\pi}}\int d\sigma\, e^{-\frac{1}{2}|\Lambda|\sigma^2+s\sigma\Lambda\hat{\Theta}}, \tag{37}$$

where $s = \pm 1$ if $\Lambda \geq 0$ or $\pm i$ if $\Lambda < 0$ and σ is the associated auxiliary field. Setting $\Lambda = -\beta V_\alpha$, we have

$$e^{-\beta\hat{H}} = \int \mathcal{D}[\sigma]G(\sigma)\, e^{-\beta\hat{h}(\sigma)}, \tag{38}$$

where $G(\sigma) = \exp(-\frac{1}{2}\beta\sum_\alpha|V_\alpha|\,\sigma_\alpha^2)$ is the Gaussian factor, the volume element is $\mathcal{D}[\sigma] = \prod_\alpha d\sigma_\alpha\sqrt{\beta\mid V_\alpha\mid/2\pi}$, and $\hat{h}(\sigma) = \sum_\alpha(\varepsilon_\alpha + s_\alpha V_\alpha\sigma_\alpha)\hat{\Theta}_\alpha$. Since in general the operators $\hat{\Theta}_\alpha$ do not commute, we split $e^{-\beta\hat{H}}$ into N_t time-slices, i.e., $e^{-\beta\hat{H}} = [e^{-\Delta\beta\hat{H}}]^{N_t}$ (all calculations presented here are with $\Delta\beta = 1/32$ MeV^{-1}) and apply the HS transformation at each time slice. Eqs. (34)-(35) can then be written as

$$\langle\hat{\Omega}\rangle = \frac{\int\mathcal{D}[\sigma]W(\sigma)\langle\hat{\Omega}\rangle_\sigma}{\int D[\sigma]W(\sigma)}. \tag{39}$$

Defining the one-body imaginary-time propagator as

$$U_\sigma = e^{-\Delta\beta h(\sigma(N_t))}\cdots e^{-\Delta\beta h(\sigma(1))} \tag{40}$$

we express the weight function $W(\sigma)$ and $\langle\hat{\Omega}\rangle_\sigma$ as

$$W(\sigma) = G(\sigma)\mathrm{Tr}_{(Z,N)}\left[U_\sigma\right], \quad \langle\hat{\Omega}\rangle_\sigma = \frac{\mathrm{Tr}_{(Z,N)}\left[\hat{\Omega}U_\sigma\right]}{\mathrm{Tr}_{(Z,N)}\left[U_\sigma\right]}. \tag{41}$$

The auxiliary fields σ_α are not just parameters introduced for numerical convenience, but have physical significance. Their presence in $\hat{h}(\sigma)$ essentially constructs a constrained mean field. Indeed, the maximum of the weight function, $W(\sigma)$, corresponds to the Hartree mean-field solution [32], satisfying the self-consistent condition

$$\sigma_\alpha^{MF} = -s_\alpha \mathrm{sgn}(V_\alpha) \langle \hat{\Theta}_\alpha \rangle_{\sigma^{MF}}. \tag{42}$$

The principal advantage of the AFMC is that overall the computational effort scales much more gently with particle number. For example, the number of proton (neutron) auxiliary fields is at most $(N_s^{p(n)})^2 \times N_t$. Thus, while for the case where $N_s^p = N_s^n = 40$ and $N_v^p = N_v^n = 20$ conventional CI methods are confronted with matrices with dimension $\sim 10^{20}$, the number of AFMC fields with $N_t = 100$ is 320,000.

Given the large number of auxiliary fields, Eq. (39) must be evaluated using Monte Carlo methods. Thus,

$$\langle \hat{\Omega} \rangle_{MC} = \frac{1}{N} \sum_i \langle \hat{\Omega} \rangle_{\sigma_i}, \tag{43}$$

where N is the number of samples (typically 4000), and σ_i is distributed according to $W(\sigma)$. The uncertainty in the integral is then governed by the variance. Central to the Monte Carlo evaluation is that $W(\sigma)$ be positive definite. For rotationally invariant applications, the general conditions for which $W(\sigma) \geq 0$ was examined in Ref. [32], and was found to be true only for a small class of semi-realistic interactions, such as pairing-plus-quadrupole, for even-particle systems. Without a positive-definite weight function, we can try to proceed by sampling with $|W(\sigma)|$. Eq. (43) is modified by the presence of the "sign", $\Phi(\sigma_i) = W(\sigma_i)/|W(\sigma_i)|$, multiplying $\langle \hat{\Omega} \rangle_{\sigma_i}$, and is normalized by the average sign $\langle \Phi \rangle$. Fig. 1 demonstrates how AFMC fails for general Hamiltonians. The figure shows the thermal energy as a function of β for ^{28}Mg within the *sd*-shell using the realistic Hamiltonian of Wildenthal [33]. The solid line shows the exact CI result, where all 28,503 eigenvalues were obtained. The circles show the AFMC calculation while sampling $|W(\sigma)|$ with the Metropolis algorithm [34]. In general, sampling with $|W(\sigma)|$ breaks down for $\beta \geq 0.4$ MeV^{-1}.

Fig. 8. Thermal energy for the nucleus ^{28}Mg computed with the *sd*-shell Hamiltonian of Wildenthal. The solid line shows the exact CI result obtained from all 28,503 shell-model eigenvalues. The (blue) circles show the AFMC result using Metropolis sampling on $|W(\sigma)|$. The (red) triangles show the results obtained using the shifted-contour method.

To address the sign problem, rewrite the two-body Hamiltonian as

$$\sum_\alpha V_\alpha \hat{\Theta}_\alpha^2 = \sum_\alpha V_\alpha (\hat{\Theta}_\alpha - \bar{\sigma}_\alpha)^2 + V_\alpha (2\hat{\Theta}_\alpha \bar{\sigma}_\alpha - \bar{\sigma}_\alpha^2), \tag{44}$$

and apply the HS transformation to the quadratic $(\hat{\Theta} - \bar{\sigma})^2$ terms, giving for $e^{-\Delta\beta \hat{H}}$

$$\int \mathcal{D}[\sigma] e^{-\frac{1}{2}\Delta\beta \sum_\alpha |V_\alpha| \sigma_\alpha^2 - V_\alpha (2 s_\alpha \sigma_\alpha \bar{\sigma}_\alpha + \bar{\sigma}_\alpha^2)} e^{-\Delta\beta \hat{h}(\sigma)}, \tag{45}$$

where now $\hat{h}(\sigma) = \sum_\alpha [\varepsilon_\alpha + V_\alpha (s_\alpha \sigma_\alpha + \bar{\sigma}_\alpha)] \hat{\Theta}_\alpha$. With the shift $\bar{\sigma}_\alpha$, the maximum of the weight function is now

$$\sigma_\alpha = -s_\alpha \mathrm{sgn}(V_\alpha)(\langle \hat{\Theta}_\alpha \rangle_\sigma - \bar{\sigma}_\alpha). \tag{46}$$

Thus, if we choose $\bar{\sigma}_\alpha = \sigma_\alpha^{MF}$, the maximum of the weight function occurs at $\sigma_\alpha = 0$. The presence of $\bar{\sigma}_\alpha$ in the exponential factors in Eq. (45) is important. For $V_\alpha < 0$, $W(\sigma)$ is shifted to the origin. While for $V_\alpha > 0$, the overall maximum is shifted into the complex plane with the maximum along the real axis at $\sigma_\alpha = 0$. Further, a static phase is introduced that suppresses the bad sign as we sample the along the real axis.

Since the maximum of $W(\sigma)$ is centered about $\sigma_\alpha = 0$ we can sample the σ-fields with the overall Gaussian factor $G(\sigma)$. The advantage of sampling with the Gaussian factor is that it offers an efficient method to sample uncorrelated values σ_i. In Fig. 9, the results of AFMC calculation of the thermal energy for ^{28}Mg using the shifted-contour method with Gaussian sampling is shown (triangles) and compared to the exact CI result as well as with Metropolis sampling on $|W(\sigma)|$. Shifting the contour yields agreement with the exact thermal calculation, which clearly represents a significant improvement over previous capability. With the zero-temperature formalism, at $\beta = 3.0$ MeV^{-1} we compute a GS energy of -120.370(25) MeV, which is in good agreement with the CI result of -120.532 MeV.

In Fig. 10, we show results for the more challenging case of ^{56}Fe, where the GXPF1A interaction [35] was used in an active model space comprised of the $0f - 1p$ orbits. Here, $N_s^{p(n)} = 20$, $N_v^p = 6$, and $N_v^n = 14$, and the number of CI basis states with $J_z = 0$ is $\approx$ 501M. Here, the GS energy is represented by the solid line in the figure. The shifted-contour AFMC calculation is clearly converging to the full-space CI result. With the zero-temperature formalism we calculate a GS energy of -195.687(107) MeV, which is in good agreement with the CI result of -195.901 MeV. The computational advantage of AFMC for large model spaces is evident as the zero-temperature calculation for ^{56}Fe took 12 CPU hours, as opposed to 1000 CPU hours for CI. The state density (the total density of states including the $(2J+1)$ degeneracy for each state of angular momentum J) can be computed with the saddle-point approximation for the inverse Laplace transform of the partition function, i.e.,

$$\rho(E) = e^{\ln Z(\beta) + \beta E(\beta)} / \sqrt{-2\pi \partial E(\beta)/\partial \beta}, \tag{47}$$

where $\ln Z(\beta) = -\int_0^\beta d\beta' E(\beta') + \ln Z(0)$, and $Z(0)$ is the total number of states given by Eq. (2). In the upper panel, we compare the calculated state density with values inferred in recent experiments [36,37]. Overall agreement with the inferred experimental quantities is achieved. Here, our intent is to demonstrate a new capability, thus our AFMC calculation consists of just one major shell. Consequently, negative-parity and higher-lying states are outside this model space, and the calculated state density will under predict the observed state density at higher excitation energies. In principal, there are no underlying computational difficulties in extending our calculations to include more major shells; only the question of the appropriate effective interaction. These results demonstrate a new capability where a fully microscopic description of the density of states is now viable.

Fig. 9. Thermal energy and the state density $\rho(E)$ for the nucleus ^{56}Fe computed with the GXPF1A fp-shell Hamiltonian. The solid line in the bottom panel shows the exact CI result for GS energy. The circles show the AFMC result using the shifted-contour method. In the upper panel, the calculated state is compared with values inferred from recent experiments [(squares) [36], (triangles) [37]].

In this section, a solution to the sign problem for the AFMC method applied to many-body systems based on shifting the quadratic part of the two-body Hamiltonian was presented. The optimal choice for the shift is the fields associated with the Hartree mean-field solution for each specific value of β. This choice shifts the maximum of the integrand to the origin; permitting efficient sampling using the Gaussian factor. For bad sign components of the Hamiltonian, the shift introduces phases that mitigate the presence of negative signs in the weight function as the fields are sampled along the real axis. With $\Delta\beta = 1/32$ MeV^{-1}, the thermal energy is typically reproduced at the level of 300 keV or better, while the GS energies are reproduced to within 150-200 keV. This is a substantial improvement over previous attempts [38], where deviations of the order 1 MeV from CI results were common [39]. However, this is also generally the level of accuracy that can achieved with the effective interactions themselves [33,35]. If the solution to the sign is as robust as it appears, the AFMC method will have wide ranging applications within the traditional CI community. Indeed, it may be possible to extend upon the earlier shell-model Hamiltonians for the sd- and fp-shells used here for heavier nuclei where the full gsd model space would be required. In this case, the number of basis states would indeed approach

10^{20}, which is well beyond the capability of any computer that will be available within the next decade. While the AFMC method is not well suited for three-body interactions, as this would necessitate a double Hubbard-Stratonovich transformation, an exciting possibility for the future is to combine the AFMC with traditional mean-field approaches based on Skyrme-like [40], Gogny, or some non-local two-body interactions. In this way, we may be able to develop a more universal picture for nuclei where one could combine for the first time the underlying physics of the mean field with the power of configuration interaction methods to arrive at a comprehensive theory of nuclei that includes the full range of quantum correlations.

6 Conclusions

In these lectures, I demonstrated the utility of configuration interaction methods and how they provide a powerful tool to describe the properties of quantum many-body systems. In particular, they offer a method to obtain first-principals solutions for the properties of light nuclei. We now know that the three-nucleon interaction plays a very important role in determining the properties of nuclei. In addition to providing more binding energy, they are also responsible for much of what we think of us as "spin-orbit" physics in nuclei. On the other hand, it is also quite apparent that full CI methods will reach computational saturation. This is inevitable as the basis dimension increases nearly exponentially with increasing particle number. In the past year, however, a decade-old problem has been solved in the Auxiliary-field Monte Carlo (AFMC) method. While this is not a matrix-diagonalization CI method per se, it operates within the same configuration Fock space, and delivers many of the same properties. The AFMC method offers a pathway to dealing with systems whose model space dimensions exceed 10^{20}, which will be beyond the capability of matrix diagonalization methods for several decades at least. The AFMC method, however, is not well suited for three-nucleon interactions. On the other hand, the very successful interactions used in conventional shell-model calculations are only two-body in nature. Consequently, it is of the utmost importance to arrive at a better understanding of the effective interaction operating in complex nuclei. The method offered here, based on the Okubo-Lee-Suzuki transformation, is a promising avenue.

For the most part, it most be said that the tremendous success that has been achieved in the past five years in nuclear theory is largely due to the advent of powerful computer platforms that have been deployed world-wide. In my opinion, the prospects for the near future are very bright, as even more powerful systems, approaching hundreds of terra-flops in performance will be readily available to the research community. From what I have seen recently, there is a new energy and a sense of optimism in nuclear theory that has not been seen in several years.

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